# Monte Carlo Simulations of Vector Spin Glasses at Low Temperatures

# Helmut G. Katzgraber

Department of Physics, University of California, Santa Cruz, CA 95064

#### Abstract

In this paper I report results for simulations of the three-dimensional gauge glass and the four-dimensional XY spin glass using the parallel tempering Monte Carlo method at low temperatures for moderate sizes. The results are qualitatively consistent with earlier work on the three- and four-dimensional Edwards-Anderson Ising spin glass. I find evidence that large-scale excitations may cost only a finite amount of energy in the thermodynamic limit. The surface of these excitations is fractal, but I cannot rule out for the XY spin glass a scenario compatible with replica symmetry breaking where the surface of low-energy large-scale excitations is space filling.

 $Key\ words\colon$  spin glasses, Frustrated Systems, parallel tempering Monte Carlo PACS: 75.50.Lk, 75.40.Mg, 05.50.+q

There has been an ongoing controversy regarding the spin glass phase. There are two main theories: the "droplet picture" (DP) by Fisher and Huse [1] and the replica symmetry breaking picture (RSB) by Parisi [2]. While RSB follows the exact solution of the Sherrington-Kirkpatrick model and predicts that excitations involving a finite fraction of the spins cost a finite energy in the thermodynamic limit, the droplet picture states that a cluster of spins of size l costs an energy proportional to  $l^{\theta}$  where  $\theta > 0$ . It follows that in the thermodynamic limit, excitations that flip a finite cluster of spins cost an infinite energy. In addition, the DP states these excitations are fractal with a fractal dimension  $d_s < d$ , where d is the space dimension, whereas in RSB these excitations are space filling, i.e.  $d_s = d$ . Krzakala and Martin, as well as Palassini and Young [3] (referred to as KMPY)

find, on the basis of numerical results on small systems with Ising symmetry, that an intermediate picture may be present: while the surface of large-scale excitations appears to be fractal, only a finite amount of energy is needed to excite them in the thermodynamic limit.

The differences between DP and RSB can be quantified by studying the distributions P(q) and  $P(q_l)$  of the spin overlap q and link overlap  $q_l$ . For finite systems, the DP predicts two peaks at  $\pm q_{\rm EA}$ , where  $q_{\rm EA}$  is the Edwards-Anderson order parameter, as well as a tail down to q=0 that vanishes in the thermodynamic limit, like  $\sim L^{-\theta}$  for perturbations introduced by a change in boundary conditions  $^1$ . In contrast, RSB predicts a non-trivial distribution with a finite weight in the tail down

<sup>&</sup>lt;sup>1</sup> In this work I use  $\theta'$  instead of  $\theta$  as I introduce the excitations thermally with *fixed* boundary conditions [6].

to q = 0, independent of system size. In addition, DP predicts the variance of the link overlap to fit a power law of the form

$$Var(q_l) = a + bL^{-\mu_l} \tag{1}$$

where a = 0 and, as shown in Ref. [6],  $\mu_l = \theta' + 2(d - d_s)$ , whereas for RSB one expects a > 0.

While there has been considerable work on Ising-type spin glass systems, only few attempts [4,5] to understand the nature of the spin glass phase for models with a vector order parameter have been made. In this work I review recent results for the three-dimensional (3D) gauge glass and the four-dimensional (4D) XY spin glass.

The Hamiltonian of the vector models analyzed can be summarized by

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij} \cos(\phi_i - \phi_j - A_{ij}), \tag{2}$$

where the sum ranges over nearest neighbors on a hypercubic lattice in d dimensions of size  $N=L^d$ . Here  $\phi_i$  represent the angles of the XY spins as  $\mathbf{S}=(\cos(\phi),\sin(\phi))$  and therefore  $|\mathbf{S}|=1$ . Periodic boundary conditions are applied. In the case of the gauge glass, I set d=3 and  $J_{ij}=1$  for all i,j. The  $A_{ij}$  are quenched random variables uniformly distributed between  $[0,2\pi]$  representing the line integral of the vector potential directed from site i to site j. For the 4D XY spin glass I set d=4 and  $A_{ij}=0$  for all i,j. The  $J_{ij}$  are chosen according to a Gaussian distribution with zero mean and standard deviation unity.

The spin overlap q is traditionally defined as

$$q = \frac{1}{N} \sum_{i=1}^{N} \mathbf{S}_{i}^{\alpha} \cdot \mathbf{S}_{i}^{\beta} , \qquad (3)$$

where  $\alpha$  and  $\beta$  represent two replicas of the system with the same disorder. For this quantity to be a sensible order parameter, it has to be maximized with respect to all symmetries of the Hamiltonian. This is described in more detail in Refs. [4] and [5] for the gauge glass and XY spin glass, respectively. In addition I introduce the link overlap  $q_l$  defined by

$$q_l = \frac{1}{N_b} \sum_{\langle i,j \rangle} (\mathbf{S}_i^{\alpha} \cdot \mathbf{S}_j^{\alpha}) (\mathbf{S}_i^{\beta} \cdot \mathbf{S}_j^{\beta}) , \qquad (4)$$

with  $N_b = dN$  the number of bonds.

To avoid critical effects influencing the data, I perform the simulations at low temperatures, typically  $T \leq 0.2T_c$ . To equilibrate the systems at such low temperatures, I use the parallel tempering Monte Carlo method [7]. For equilibration tests for parallel tempering Monte Carlo on the models studied I refer the reader to Refs. [4] and [5].

#### Results

Figures 1 and 2 show data  $^2$  for P(|q|) and  $P(q_l)$  at T=0.050, well below  $T_c\approx 0.45$  [8] for the 3D gauge glass.

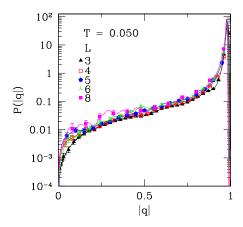


Fig. 1. Data for the overlap distribution P(|q|) at temperature T=0.050 for the 3D gauge glass. Note the logarithmic vertical scale. In this and other similar figures in the paper, I only display a subset of all the data points while the lines connect all the data points in the set. Thus, the structure in the lines between neighboring symbols is meaningful.

There is a clear peak in P(|q|) for large |q| as well as a tail at small |q|. The weight in the tail does not decrease with increasing L, as is expected in the standard interpretations of the droplet theory. If anything, the weight increases for larger sizes. There is some evidence that P(|q|) stays flat down to smaller |q| for larger L, although the range of sizes is too small to make a reliable extrapolation.

<sup>&</sup>lt;sup>2</sup> I present data for |q| since for the gauge glass  $q \in \mathbb{C}$ .

As with the distribution of |q|, there is a pronounced peak at large  $q_l$ -values in the distribution of  $P(q_l)$  for the 3D gauge glass. Note also the appearance of a smaller peak at smaller  $q_l$  for larger system sizes, as predicted by RSB.

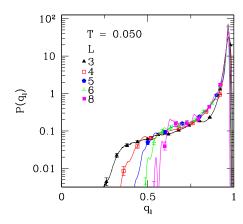


Fig. 2. The distribution of the link overlap at T=0.050 for the 3D gauge glass. Note the logarithmic vertical scale.

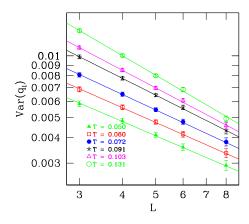


Fig. 3. Log-log plot of the variance of  $q_l$  vs. L at several temperatures for the 3D gauge glass.

The width of the distribution decreases with increasing system size. This can be seen in Figure 3 where I plot the variance of the link overlap as a function of system size L. The data is consistent with a power law decrease (a = 0 in Eq. 1) where the (presumably effective) exponent varies slightly with T. Extrapolating to T = 0 gives  $\mu_l \equiv$ 

 $\theta' + 2(d - d_s) = 0.501 \pm 0.04$ . Assuming  $\theta' \approx 0$  I find  $d - d_s = 0.25 \pm 0.02$ , implying that for the 3D gauge glass system-size excitations have a fractal surface in the thermodynamic limit as predicted by the droplet picture.

Figures 4 and 5 show data for P(q) and  $P(q_l)$  for T=0.20 (to be compared with  $T_c\approx 0.95$  [9]) for the 4D XY spin glass. Again one sees a large peak for large q and  $q_l$  values. The data for  $P(q_l)$  exhibits a hint of a shoulder for smaller values of  $q_l$ .

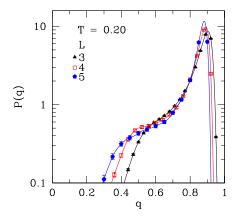


Fig. 4. Data for the overlap distribution P(q) at T=0.20 for 4D XY spin glass. Note the logarithmic vertical scale.

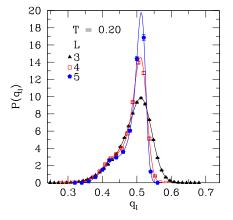


Fig. 5. The distribution of the link overlap at T=0.20 for the 4D XY spin glass.

The width of the distribution decreases with increasing system size. This is demonstrated in Fig. 6

where I show the variance of  $q_l$  against system size L for several low temperatures. There is some curvature in the data for  $Var(q_l)$  so first I attempt a three-parameter fit to Eq. 1. As there are the same number of data points as variables, I cannot assign fitting probabilities to the fits but from the data I find a = 0.00100, 0.00087, 0.00073 and 0.00036 for T = 0.200, 0.247, 0.305 and 0.420, respectively.

I also attempt a power law fit to Eq. 1 setting a=0. The quality of the fits is poor with probabilities  $Q=5.0\times 10^{-2}, 3.6\times 10^{-3}, 2.9\times 10^{-6}$  and  $6.0\times 10^{-8}$  for T=0.200, 0.247, 0.305 and 0.42, respectively <sup>3</sup>. The effective exponent  $\mu_l$  is found to vary with temperature. Extrapolating to T=0, I obtain  $\mu_l\equiv\theta'+2(d-d_s)=0.294\pm0.073$ . Assuming  $\theta'\approx 0$ , one obtains  $d-d_s=0.147\pm0.036$ .

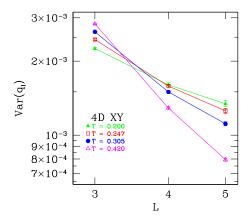


Fig. 6. Log-log plot of the variance of  $q_l$  vs. L at several temperatures for the 4D XY spin glass.

## Conclusions

To conclude, I have studied the properties of the 3D gauge glass and the 4D XY spin glass at low temperatures. For both models, the order parameter distribution P(q) has, in addition to a peak, a tail that seems to extend for smaller values of q and whose height seems to persist as the system size increases. This interpretation of the data

is compatible with the RSB picture or the KMPY scenario. The range of lattice sizes is very small, however, so this conclusion can be considered at most tentative.

For the gauge glass, the variance of the link overlap indicates that the surface of low-energy large-scale excitations is fractal with  $d - d_s =$  $0.25 \pm 0.02$  in agreement with the KMPY scenario. The log-log plot for  $Var(q_l)$  for the XY spin glass shows curvature, possibly indicating a non-zero value in the thermodynamic limit, a result compatible with RSB. Due to the small range of system sizes, however, I cannot rule out the possibility that  $Var(q_l) \to 0$  at large L, which is compatible with the KMPY scenario or droplet picture. The effects of vortices in the spin glass phase still remain to be understood. It would be useful to look more carefully at the nature of the large-scale low-energy excitations to see whether they correspond to gradual orientations in the spin directions or whether vortices play a role.

I would like to thank A. P. Young for useful discussions. This work was supported by the National Science Foundation under grant DMR 0086287 and a Campus Laboratory Collaboration (CLC).

### References

- D. S. Fisher and D. A. Huse, J. Phys. A. 20 L997 (1987).
- [2] G. Parisi, Phys. Rev. Lett. 43, 1754 (1979).
- [3] F. Krzakala and O. C. Martin, Phys. Rev. Lett. 85, 3013 (2000); M. Palassini and A. P. Young, Phys. Rev. Lett. 85, 3017 (2000).
- [4] H. G. Katzgraber and A. P. Young, Phys. Rev. B 64, 104426, (2001).
- [5] H. G. Katzgraber and A. P. Young, submitted to Phys. Rev. B, (cond-mat/0108320).
- [6] H. G. Katzgraber, M. Palassini and A. P. Young, Phys. Rev. B 63, 184422, (2001).
- [7] K. Hukushima and K. Nemoto, J. Phys. Soc. Japan 65, 1604, (1996); E. Marinari, Advances in Computer Simulation, edited by J. Kertész and Imre Kondor (Springer-Verlag, Berlin 1998), p. 50.
- [8] T. Olson and A. P. Young, Phys. Rev. B 61, 12467 (2000).
- [9] S. Jain, J. Phys. A **29**, L385. (1996).

<sup>&</sup>lt;sup>3</sup> The complete set of fitting parameters for both fitting functions presented in Eq. 1 can be found in Ref. [5].